Closures for Coarse-Grid Simulation of Fluidized Gas-Particle Flows

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Ronald Breault, Project Manager

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June 5, 2007: 1:25 PM – 2:00 PM

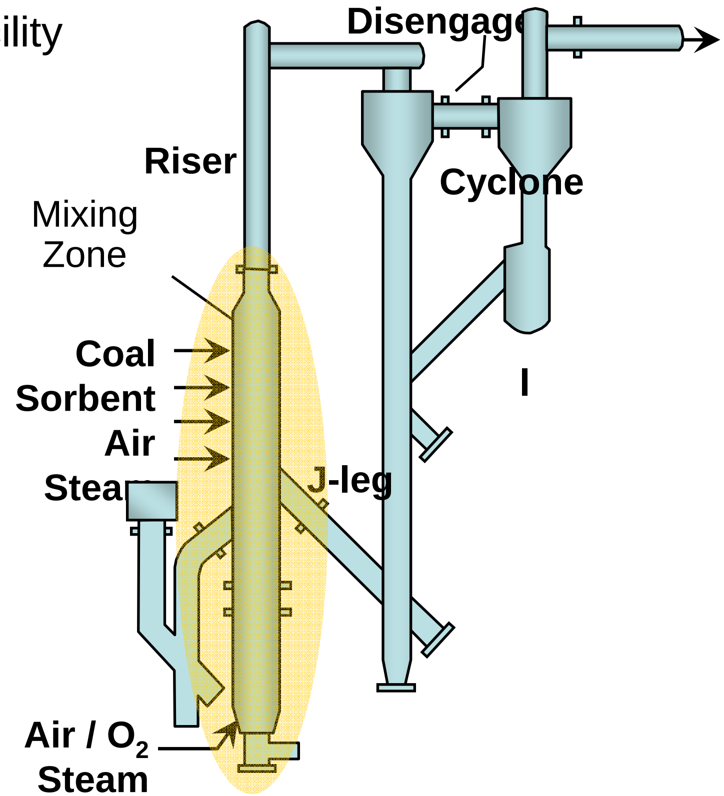
Grand Ball Room 5, Session A

Outline

- *The Problem and Project Objectives*
- *Year 1 Goals*
- *Principal results from Year 1*
- *Summary*
- *Outlook for Years 2 and 3*

Advanced Coal Gasification Technology

Power Systems Development Facility
Wilsonville, Alabama



<u>Demonstration Scale</u>

- Air and oxygen blown operation
- Coal Feed Rate ~5000 lbs/hr
- Bituminous and Sub-bituminous
- Pressure (250 psi)

<u>Commercial Scale</u>

- Air and oxygen blown operation
- Coal Feed Rate ~250,000 lbs/hr
- Bituminous and Sub-bituminous
- Pressure (465 psi)

Chris Guenther, NETL

DOE – NETL; KBR; Southern Co; Siemens – Westinghouse
Electric Power Res. Inst.; Peabody Holding Co.; Southern Res. Inst.

Characteristics of flows in turbulent fluidized beds & fast fluidized beds

- Up to ~ 30 vol% particles, with particle size distribution
- Persistent density and velocity fluctuations
  - Wide range of spatial scales
  - Wide range of frequencies
  - Macroscopically inhomogeneous structures, such as radial segregation of particles in risers (core-annular flow)
- Particle-particle collisions
- Too many particles to track individually
- Model in terms of local-average variables in locally-averaged equations of motion (“two-fluid models”)

Two-fluid model equations: uniformly sized particles

Continuity equations

Solids
$$\frac{\partial(\rho_s\phi_s)}{\partial t}+\nabla\cdot(\rho_s\phi_s\boldsymbol{u}_s)=0$$

Fluid
$$\frac{\partial(\rho_f\phi_f)}{\partial t}+\nabla\cdot(\rho_f\phi_f\boldsymbol{u}_f)=0$$

Solids
$$\frac{\partial}{\partial t}(\rho_s\phi_s\boldsymbol{u}_s)+\nabla\cdot(\rho_s\phi_s\boldsymbol{u}_s\boldsymbol{u}_s)=-\nabla\cdot\boldsymbol{\sigma}_s\quad-\phi_s\nabla\cdot\boldsymbol{\sigma}_f\quad+\boldsymbol{f}\quad+\rho_s\phi_s\boldsymbol{g}$$

inertia | solid phase stress | *effective buoyancy* | interphase interaction | *gravity*

Fluid
$$\frac{\partial}{\partial t}(\rho_f\phi_f\boldsymbol{u}_f)+\nabla\cdot(\rho_f\phi_f\boldsymbol{u}_f\boldsymbol{u}_f)=\quad-\phi_f\nabla\cdot\boldsymbol{\sigma}_f\quad-\boldsymbol{f}\quad+\rho_f\phi_f\boldsymbol{g}$$

Readily extended to binary particle mixtures

Two-fluid model equations: uniformly sized particles

Inter-phase force – due to *gas-particle drag*
(*Wen* & Yu, 1966)

Solids

$$\frac{\partial}{\partial t}\left(\rho_s\phi_s\boldsymbol{u}_s\right)+\nabla\cdot\left(\rho_s\phi_s\boldsymbol{u}_s\boldsymbol{u}_s\right)=-\nabla\cdot\boldsymbol{\sigma}_s \quad -\phi_s\nabla\cdot\boldsymbol{\sigma}_f \quad +\boldsymbol{f} \quad +\rho_s\phi_s\boldsymbol{g}$$

solid phase stress | ***effective buoyancy*** | **interphase interaction**

Fluid

$$\frac{\partial}{\partial t}\left(\rho_f\phi_f\boldsymbol{u}_f\right)+\nabla\cdot\left(\rho_f\phi_f\boldsymbol{u}_f\boldsymbol{u}_f\right)= \quad -\phi_f\nabla\cdot\boldsymbol{\sigma}_f \quad -\boldsymbol{f} \quad +\rho_f\phi_f\boldsymbol{g}$$

Two-fluid model equations: uniformly sized particles

Mass loading of particles is high and the deviatoric stress in the gas phase plays virtually no role

Solids

$$\frac{\partial}{\partial t}\left(\rho_s \phi_s \boldsymbol{u}_s\right) + \nabla \cdot \left(\rho_s \phi_s \boldsymbol{u}_s \boldsymbol{u}_s\right) = -\nabla \cdot \boldsymbol{\sigma}_s \quad - \phi_s \nabla \cdot \boldsymbol{\sigma}_f \quad + \boldsymbol{f}_{drag} \quad + \rho_s \phi_s \boldsymbol{g}$$

solid phase stress — ***effective buoyancy*** — **drag**

Fluid

$$\frac{\partial}{\partial t}\left(\rho_f \phi_f \boldsymbol{u}_f\right) + \nabla \cdot \left(\rho_f \phi_f \boldsymbol{u}_f \boldsymbol{u}_f\right) = \quad - \phi_f \nabla \cdot \boldsymbol{\sigma}_f \quad - \boldsymbol{f}_{drag} \quad + \rho_f \phi_f \boldsymbol{g}$$

Two-fluid model equations: uniformly sized particles

Model particle phase stress through the kinetic theory of granular materials – augment the system with an additional equation for the fluctuation energy

Solids

$$\frac{\partial}{\partial t}\left(\rho_s \phi_s \boldsymbol{u}_s\right) + \nabla \cdot \left(\rho_s \phi_s \boldsymbol{u}_s \boldsymbol{u}_s\right) = -\nabla \cdot \boldsymbol{\sigma}_s \quad - \phi_s \nabla p_f \quad + \boldsymbol{f}_{drag} \quad + \rho_s \phi_s \boldsymbol{g}$$

solid phase stress — *effective buoyancy* — **drag**

Fluid

$$\frac{\partial}{\partial t}\left(\rho_f \phi_f \boldsymbol{u}_f\right) + \nabla \cdot \left(\rho_f \phi_f \boldsymbol{u}_f \boldsymbol{u}_f\right) = \quad - \phi_f \nabla p_f \quad - \boldsymbol{f}_{drag} \quad + \rho_f \phi_f \boldsymbol{g}$$

e.g., see Gidaspow (1994)

Plus, boundary conditions

Solution of discretized form of the kinetic theory based two-fluid model

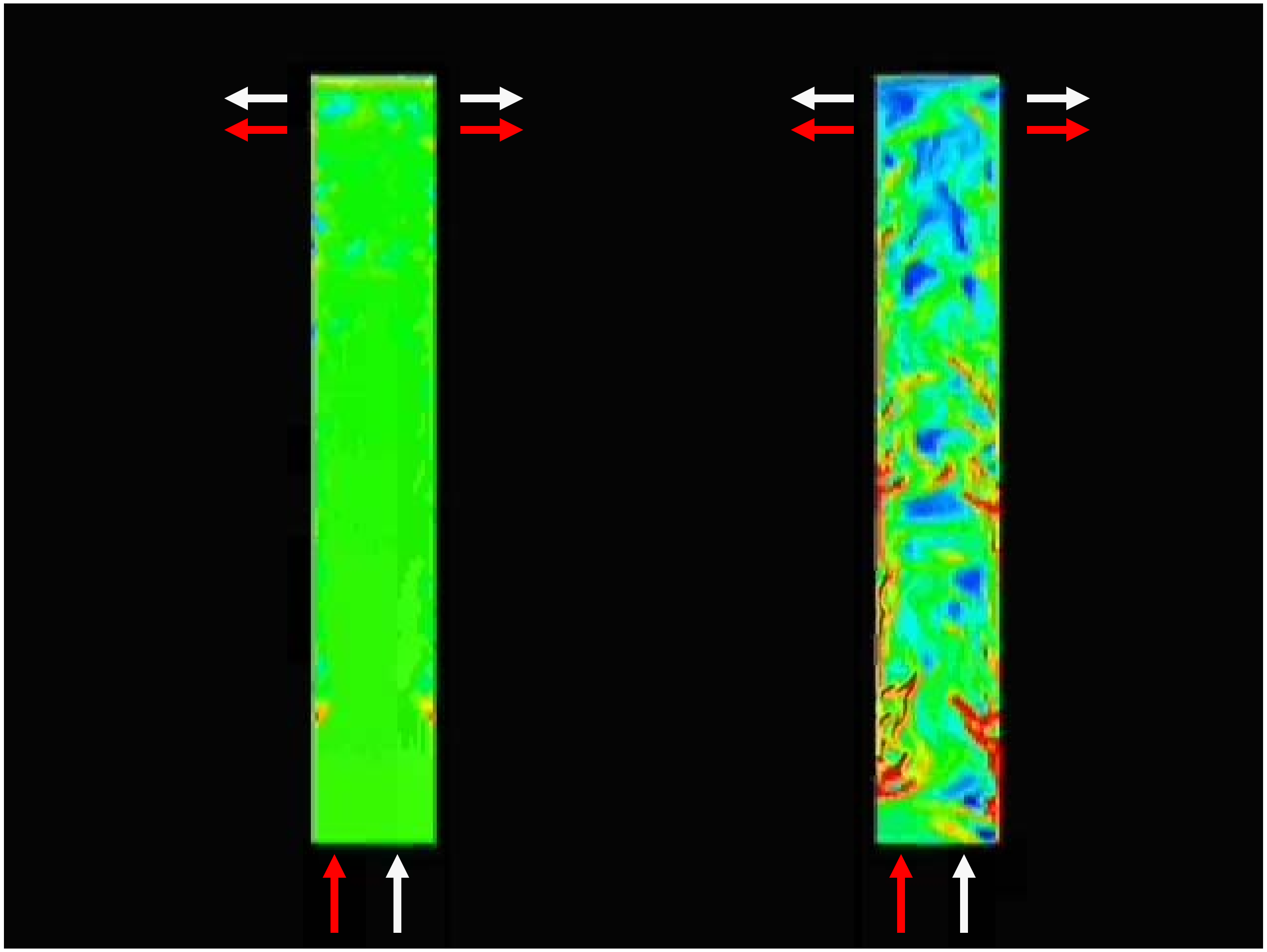
30 m tall

76 cm channel width

75μm particles

2 cm grid

2-D simulations



Gas vel = 6 m/s
Solids flux = 220 kg/m2.s

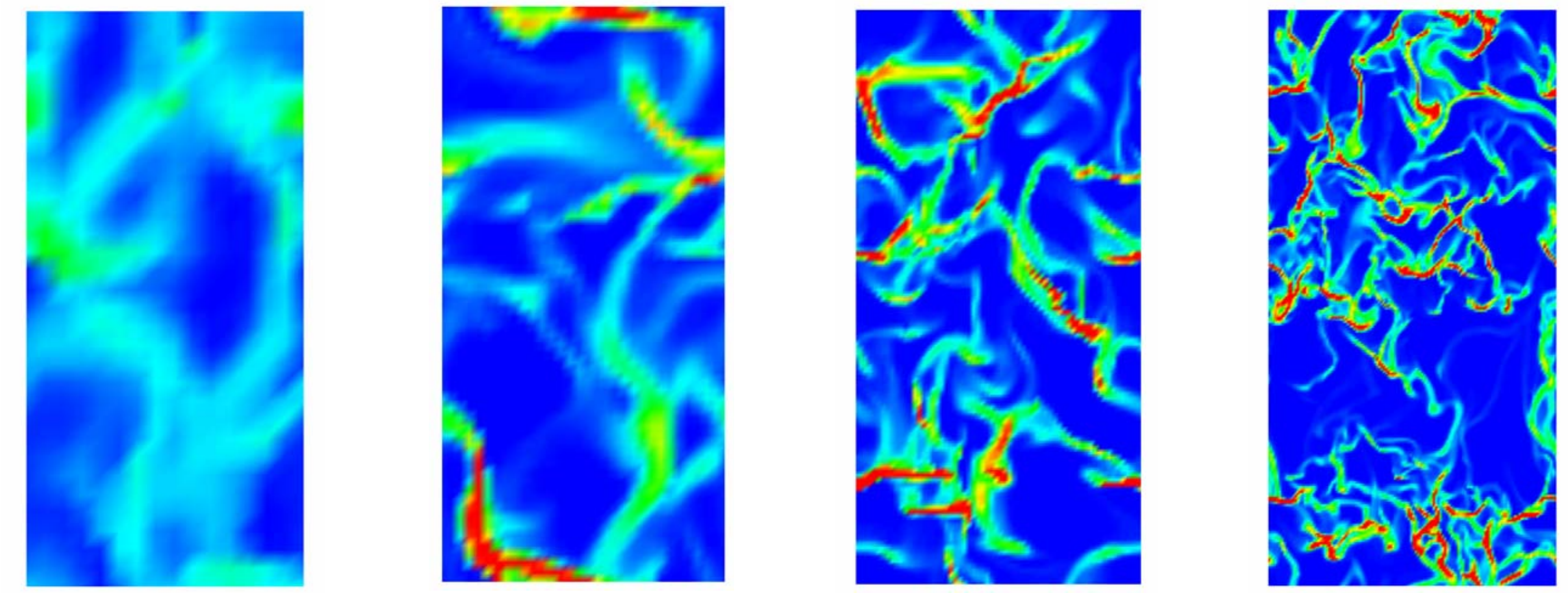
What I get

What I expect based on experimental data

FCC particles in air; 16cm x 32 cm

Simulations using MFIX {www.mfix.org}

1.0 cm | 0.500 cm | 0.250 cm | 0.125 cm



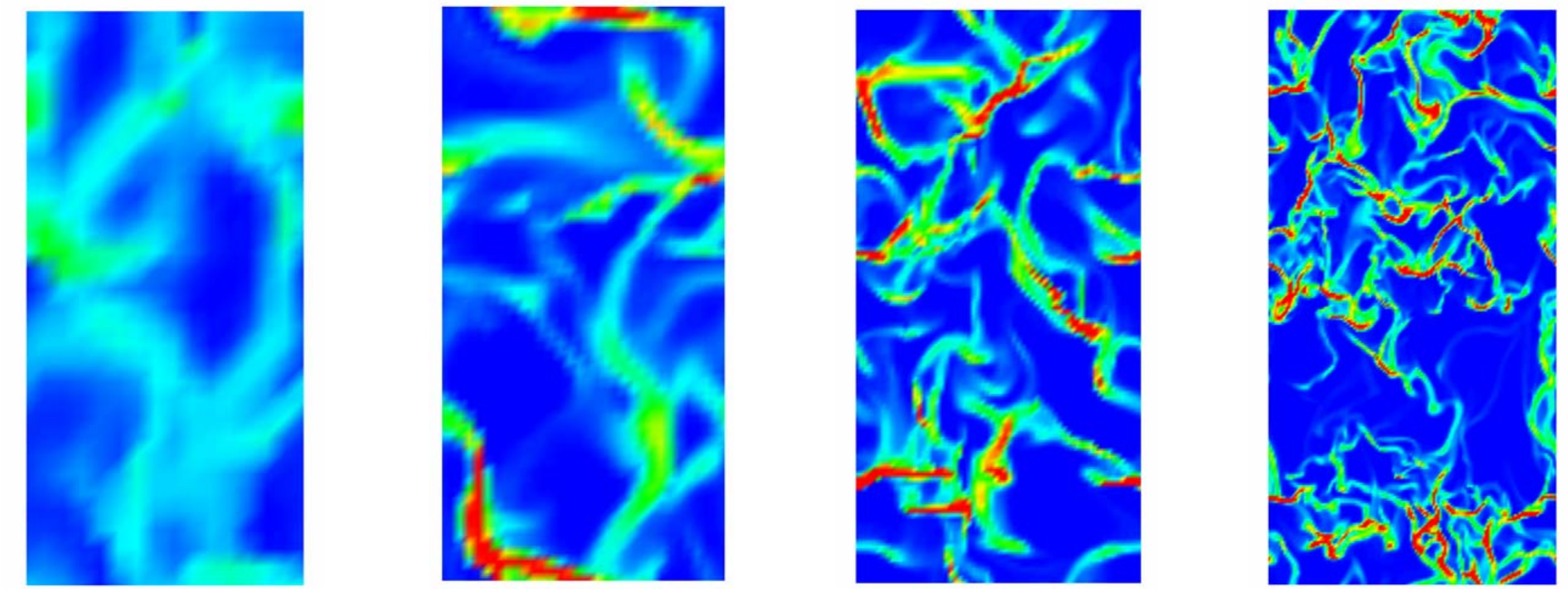
16x32 | 32x64 | 64x128 | 128x256

Snapshots of particle volume fraction fields – kinetic theory based two-fluid model. Red color indicates regions of high particle volume fractions.

FCC particles in air; 16cm x 32 cm

Simulations using MFIX {www.mfix.org}

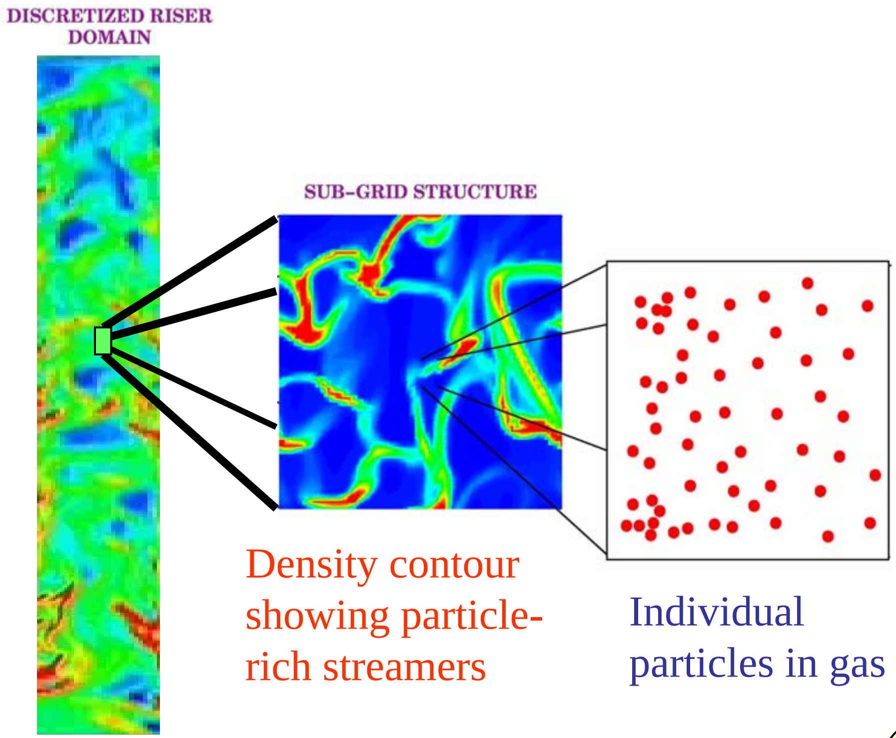
1.0 cm	0.500 cm	0.250 cm	0.125 cm



16x32	32x64	64x128	128x256

- Fine structures affect effective fluid-particle interaction force and stresses
- Do we really want to resolve them?

Project Objective: Coarse-grained equations



All the constitutive models for the two-fluid models are for nearly homogeneous mixtures

Multiphase flow computations via two-fluid models

Reaction engineering need:
Tools to probe macro-scale reactive flow features directly

Single-phase turbulent Flows

- Eddies with a wide range of length and time scales
- Too expensive to resolve all the eddies through Direct Numerical Simulation of the Navier-Stokes Equations
- Approach: Simulate the large eddies and model the smaller eddies – Large Eddy Simulations
- Filtered Navier Stokes equations
- Unresolved eddies – effective transport properties: viscosity, diffusivities

Project Objectives

Develop models that allow us to focus on large-scale flow structures, without ignoring the possible consequence of the smaller scale structures.

Original two-fluid model and constitutive relations → Filtered two-fluid model

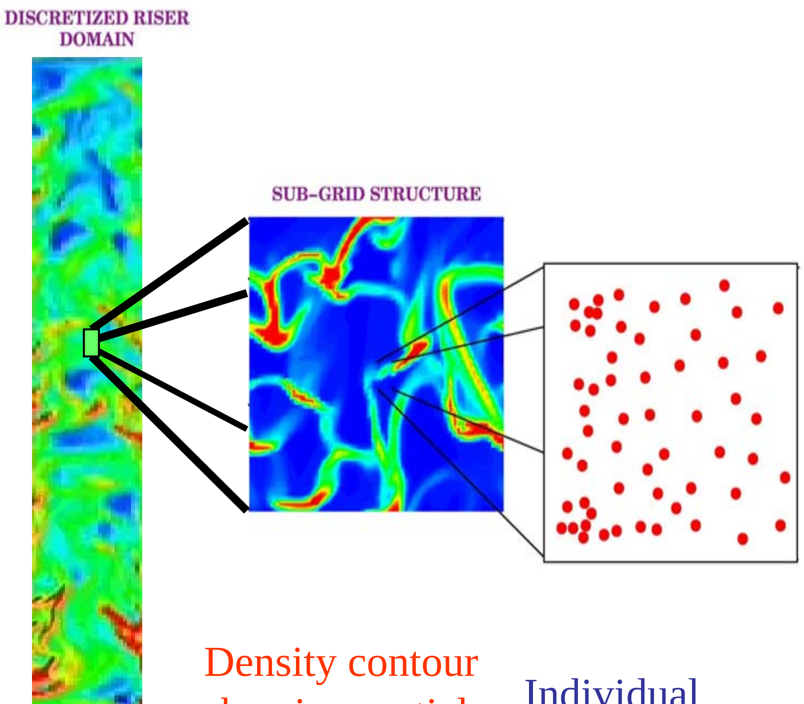
Modified constitutive relations

- Construct constitutive models that filter over meso-scale structures that occur over length scales of 100 – 1000 particle diameters
- First do for the case of uniformly sized particles; then extend to binary mixtures
- Validate filtered models

Year 1 Goals

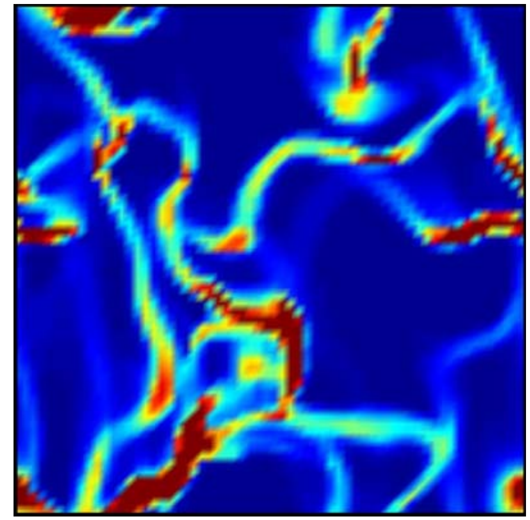
- Perform highly resolved 2-D and 3-D simulations of a kinetic theory based microscopic two-fluid model for uniformly sized particles, and construct closures for filtered drag coefficient, filtered particle phase pressure and filtered gas & particle phase viscosities.

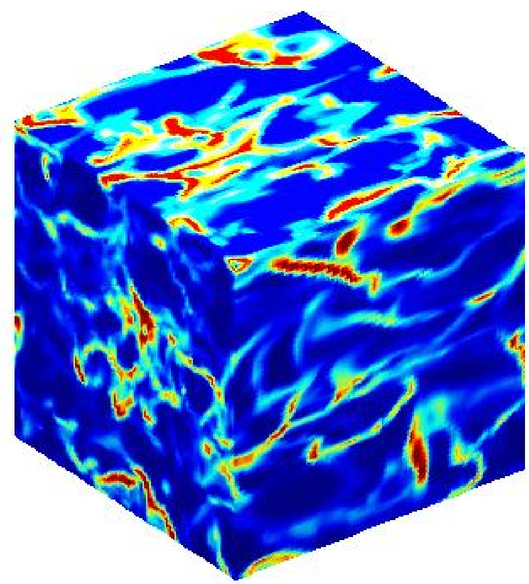
Mechanics of Gas-Particle Flows



Density contour showing particle-rich streamers

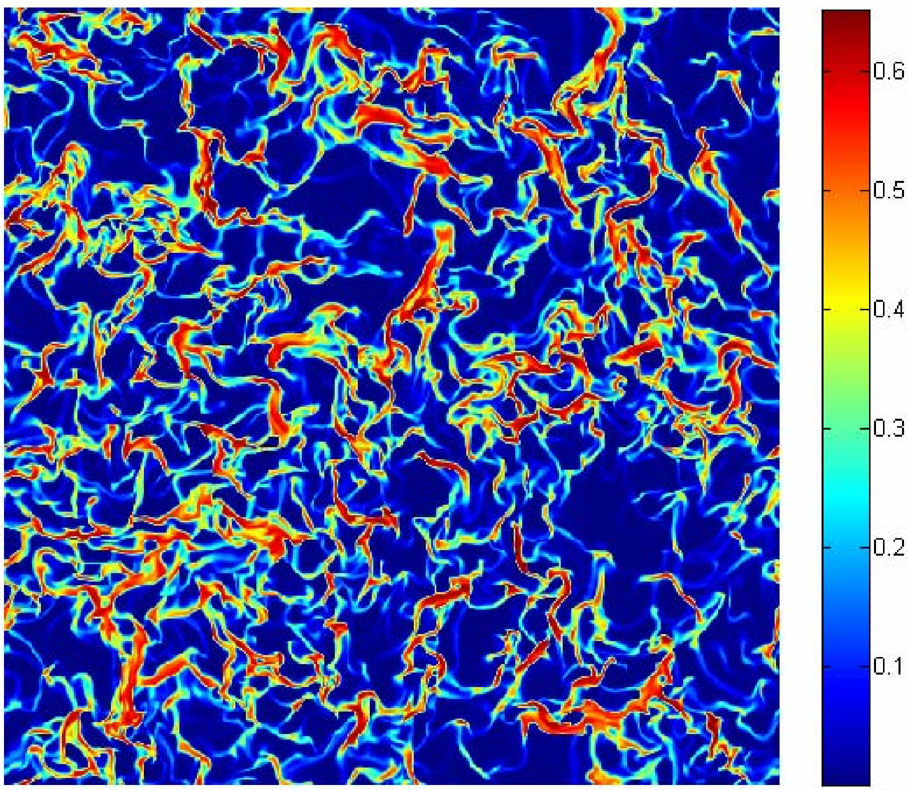
Individual particles in gas





Approach: Probe details of mesoscale structures and develop effective coarse-grained equations

Kinetic Theory Based Model



Snapshot of the volume fraction field in a 2-D simulation

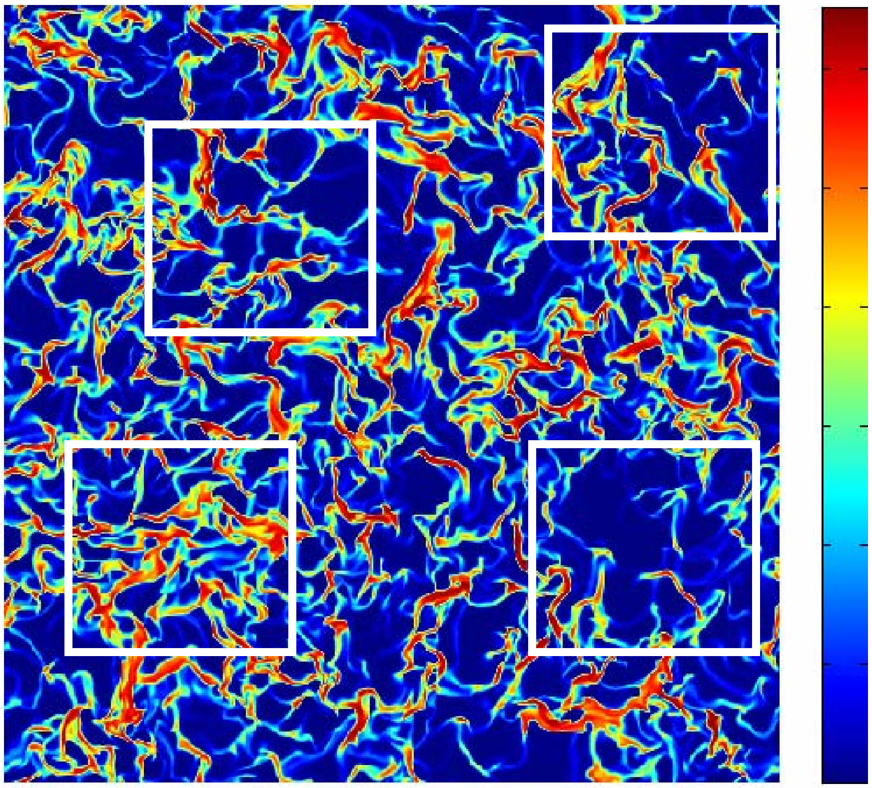
64 cm x 64 cm

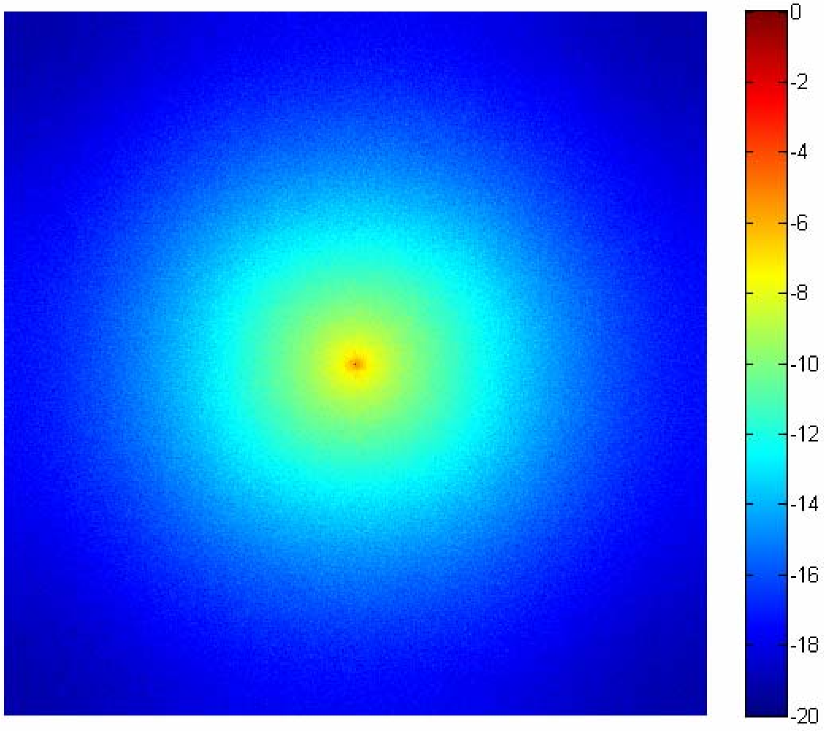
512 x 512 grids

Average volume fraction of particles = 0.15

Periodic domain with a vertical pressure gradient to balance the weight of the suspension

Kinetic Theory Based Model





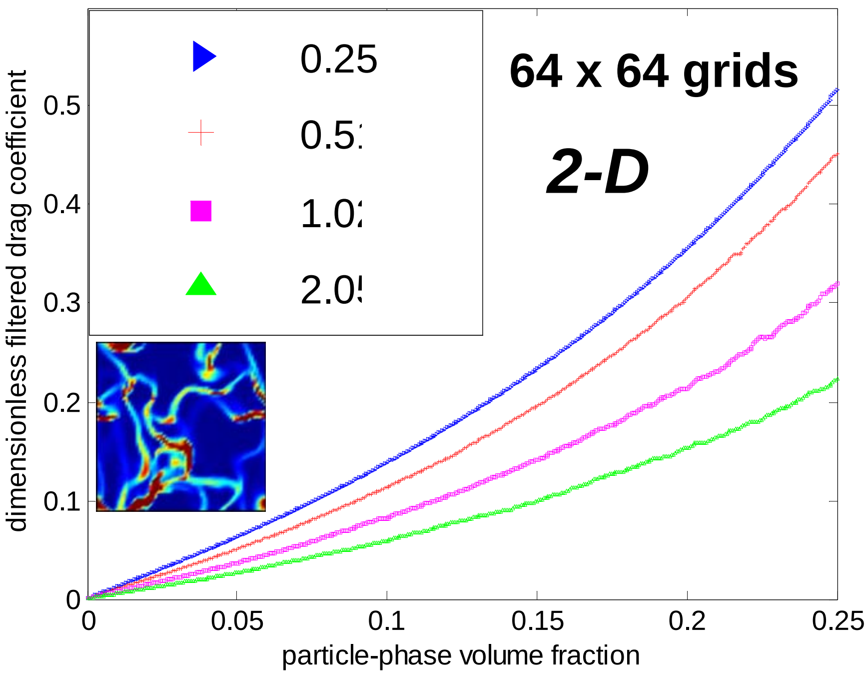
Power spectra

Meso-scale structures are statistically isotropic

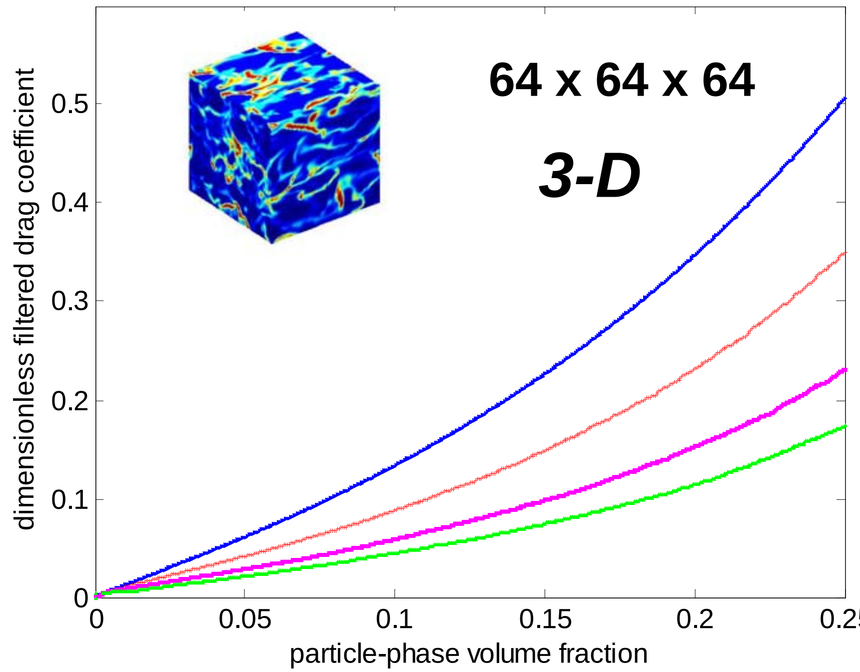
Filtered drag coefficient decreases as filter size increases for both 2-D and 3-D

$$\frac{\beta V_t}{\rho_s g}$$

Domain size = 16 x 16



16 x 16 x 16



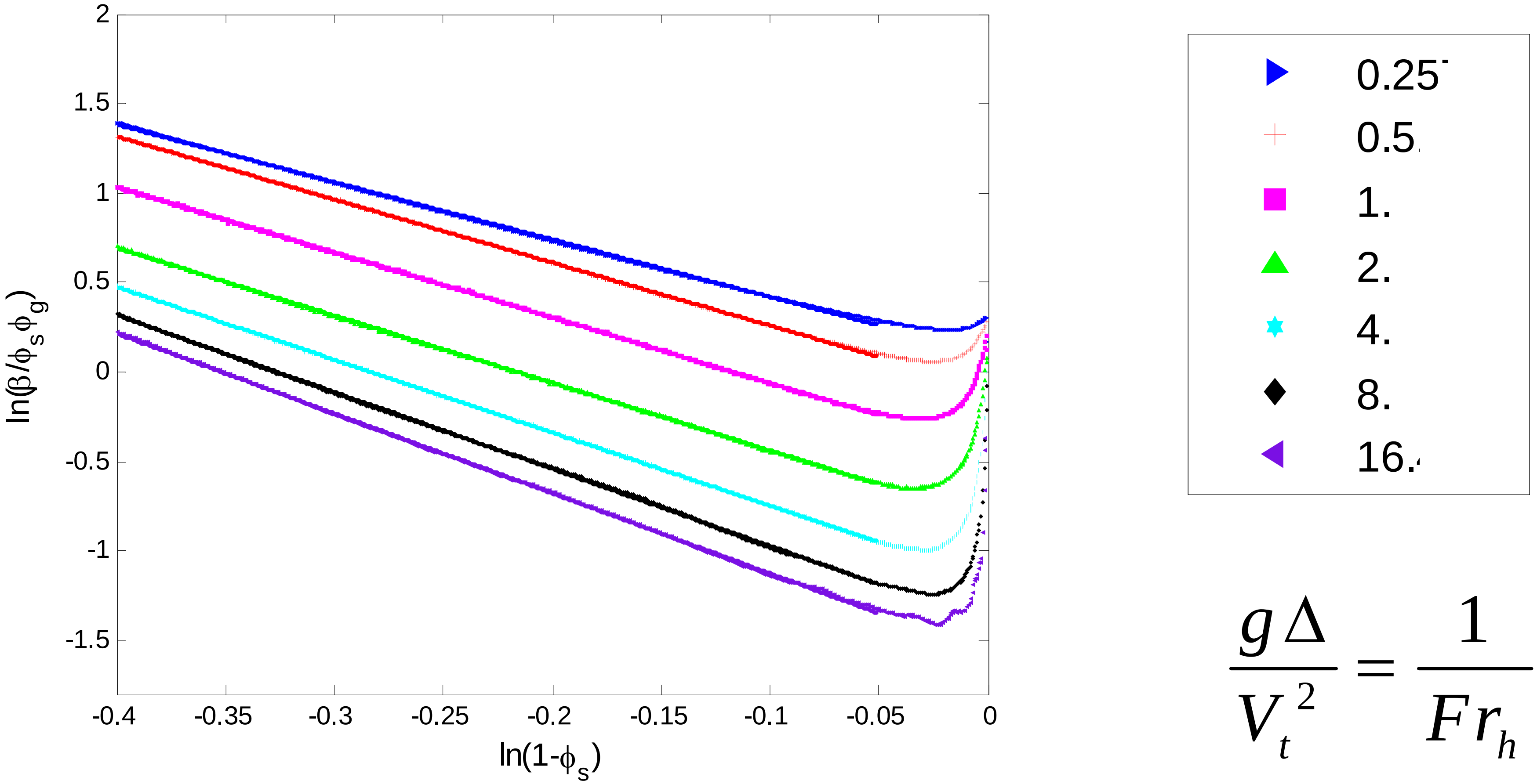
Example: 75 μm; 1500 kg/m^3; domain size = 8 cm

$$\frac{g\Delta}{V_t^{\,2}} = \frac{1}{Fr_h}$$

$$\frac{1}{Fr_h} = 2 \;\Rightarrow \Delta = 1cm$$

Variation of filtered drag coefficient with filter size 2-D

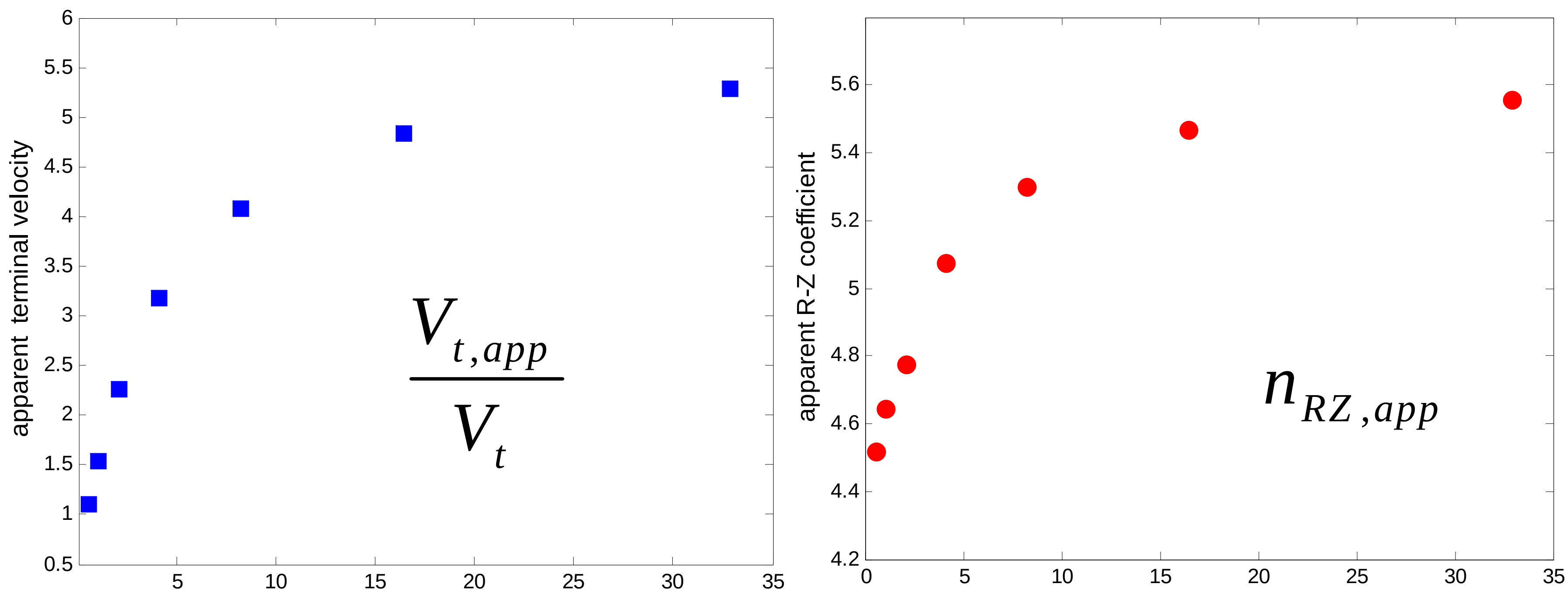
$$\frac{\beta V_t}{\rho_s g \phi_s (1-\phi_s)}$$



$$\frac{g\Delta}{V_t^{\,2}} = \frac{1}{Fr_h}$$

Filtered drag coefficient 2-D

$$\beta = \frac{\rho_s g \phi_s}{V_{t,app}\left(1-\phi_s\right)^{n_{RZ,app}-2}}$$

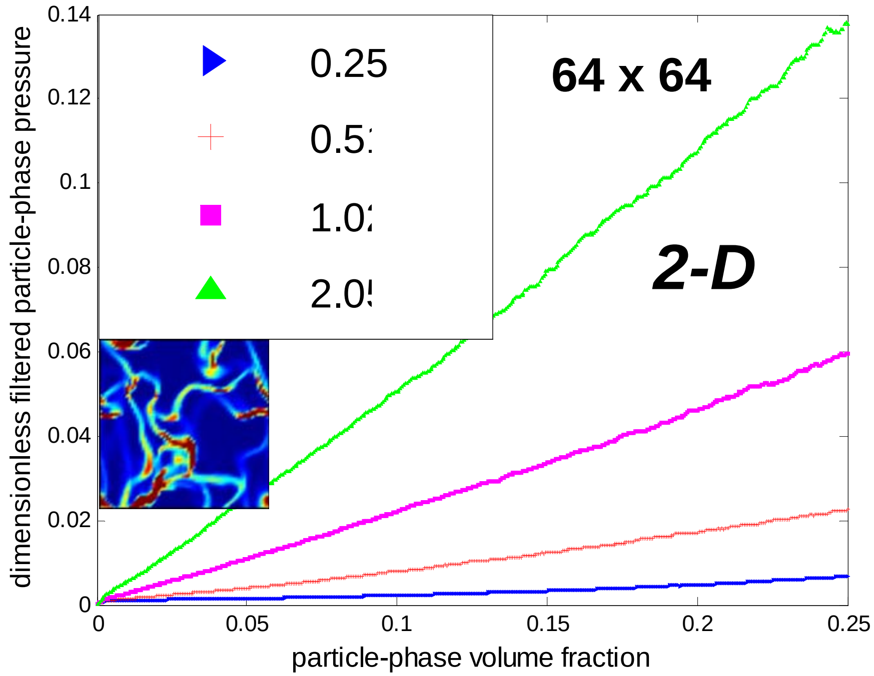


$$\frac{g\Delta}{V_t^{\,2}} = \frac{1}{Fr_h}$$

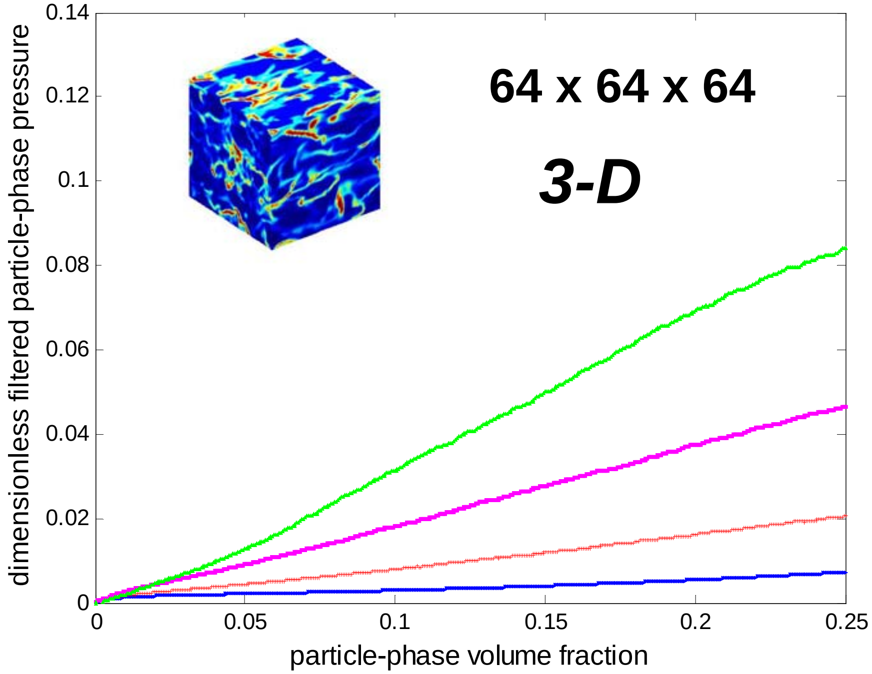
Filtered particle phase pressure increases as filter size increases for both 2-D and 3-D

$$\frac{p_s}{\rho_s V_t^2}$$

Domain size: 16 x 16



16 x 16 x 16



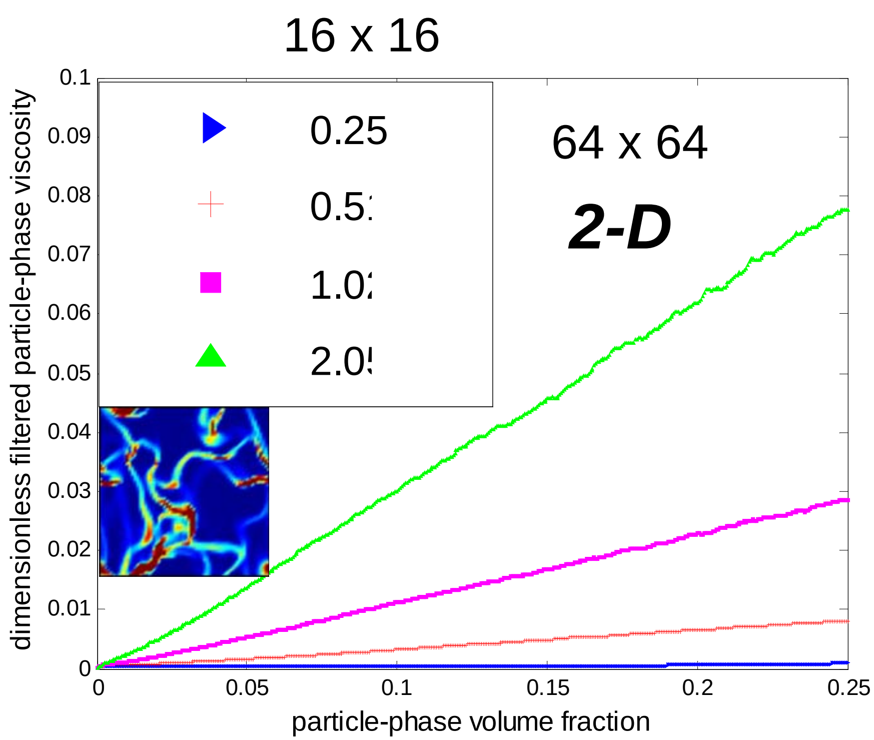
Example: 75 μm; 1500 kg/m^3; domain size = 8 cm

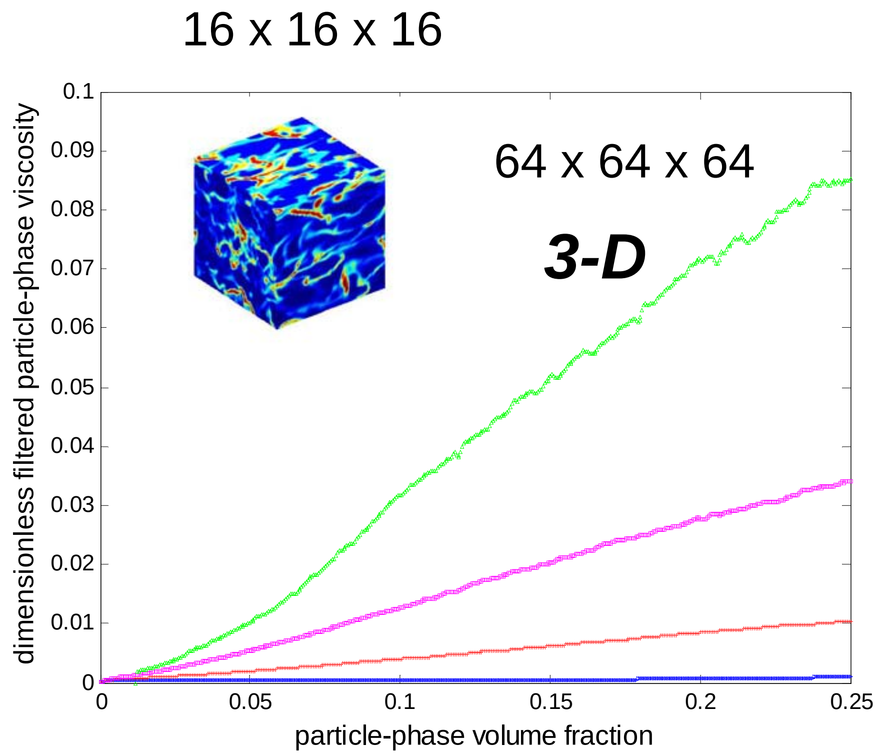
$$\frac{g\Delta}{V_t^2} = \frac{1}{Fr_h}$$

$$\frac{1}{Fr_h} = 2 \Rightarrow \Delta = 1cm$$

Filtered particle phase viscosity increases as filter size increases for both 2-D and 3-D

$$\frac{\mu_s g}{\rho_s V_t^3}$$





Example: 75 μm; 1500 kg/m^3; domain size = 8 cm

$$\frac{g\Delta}{V_t^2} = \frac{1}{Fr_h}$$

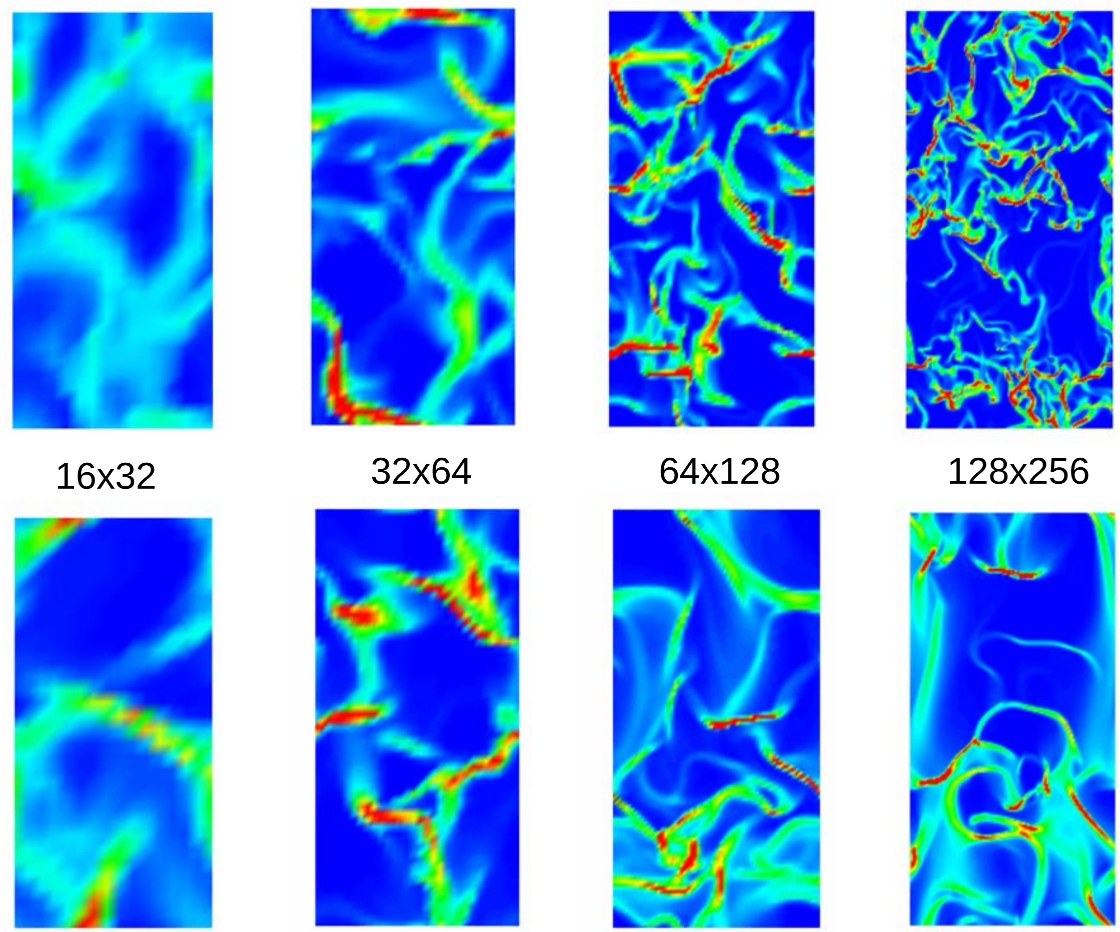
$$\frac{1}{Fr_h} = 2 \Rightarrow \Delta = 1cm$$

Comparison of the kinetic theory and filtered models

Kinetic theory based (original) two-fluid model

16x32 cm

Filtered two-fluid model

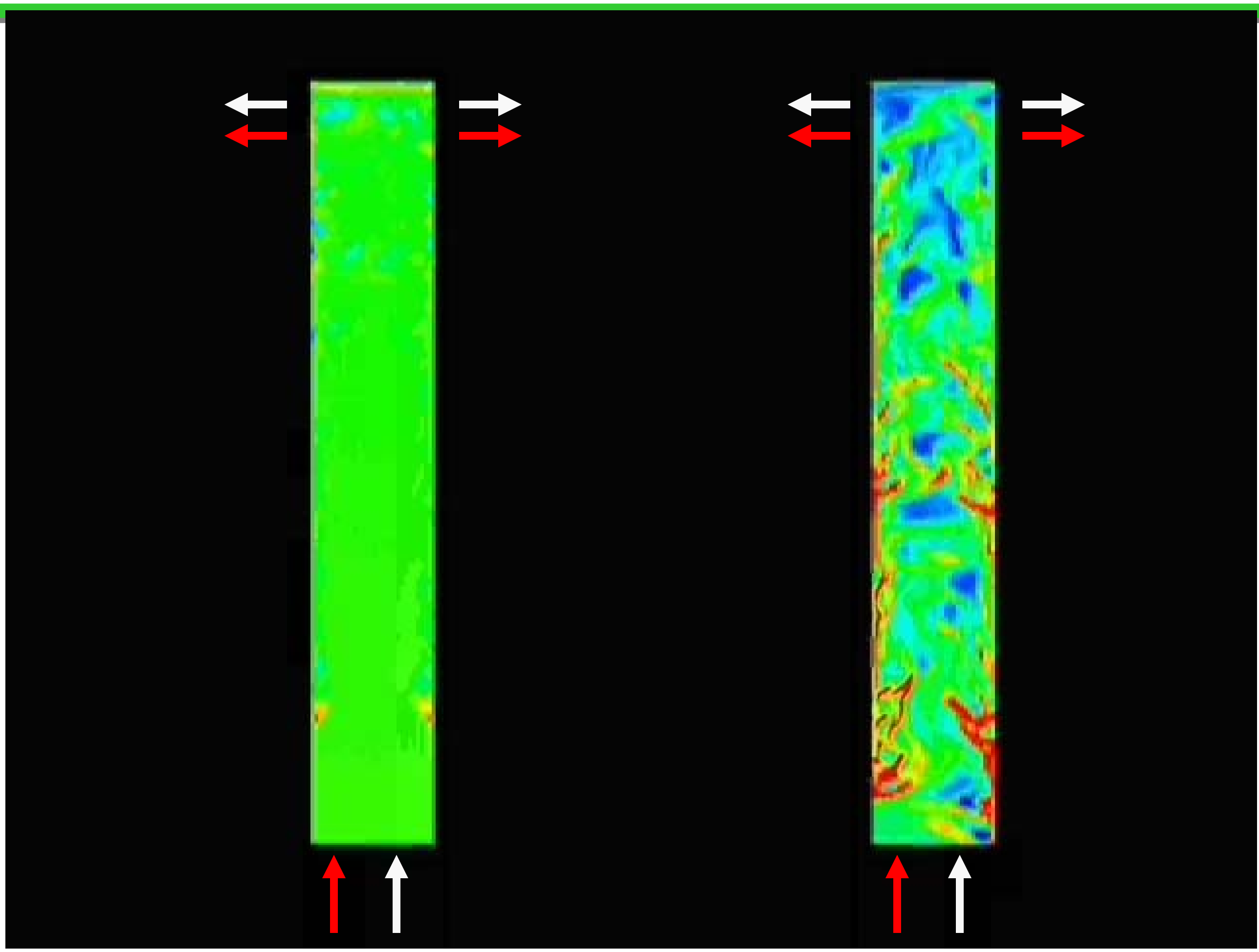


Solution of discretized form of the microscopic and the filtered equations of motion

30 m tall

76 cm channel width

2 cm grid

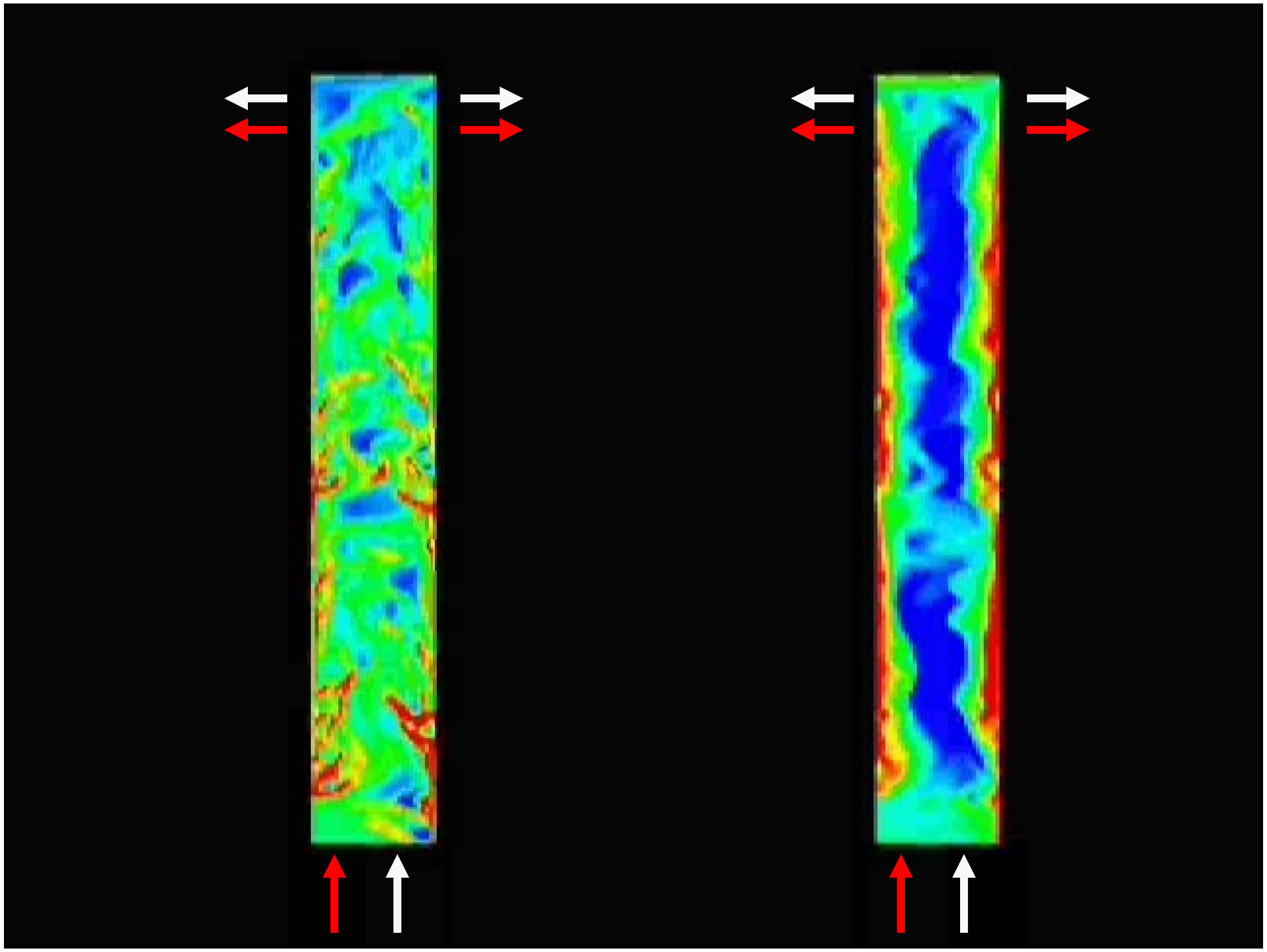


Gas velocity = 6 m/s
Solids flux = 220 kg/m2.s

Kinetic theory

Filtered equations

Solution of discretized form of the filtered equations of motion



Particle volume fraction　　　Vertical velocity

Summary

- Through highly resolved simulations of *any* two-fluid model, one can extract closures for the corresponding filtered two-fluid model. We have demonstrated this for a kinetic theory based two-fluid model.
- The drag law and the effective stresses which should be used in the filtered equations vary systematically with filter size.
- Two-dimensional and three-dimensional analyses yield similar statistical information.
- The test problem shows that the “filtered equations” approach has promise. But questions remain.

Project Goals: Years 2 and 3

- Develop scaling relations (Year 2)
- Examine the effect of bounding walls on the closures for the filtered quantities (years 2 & 3)
- Extend to binary mixtures (Years 2 and 3)
- Validate the filtered two-fluid model equations against experimental data (Year 3)

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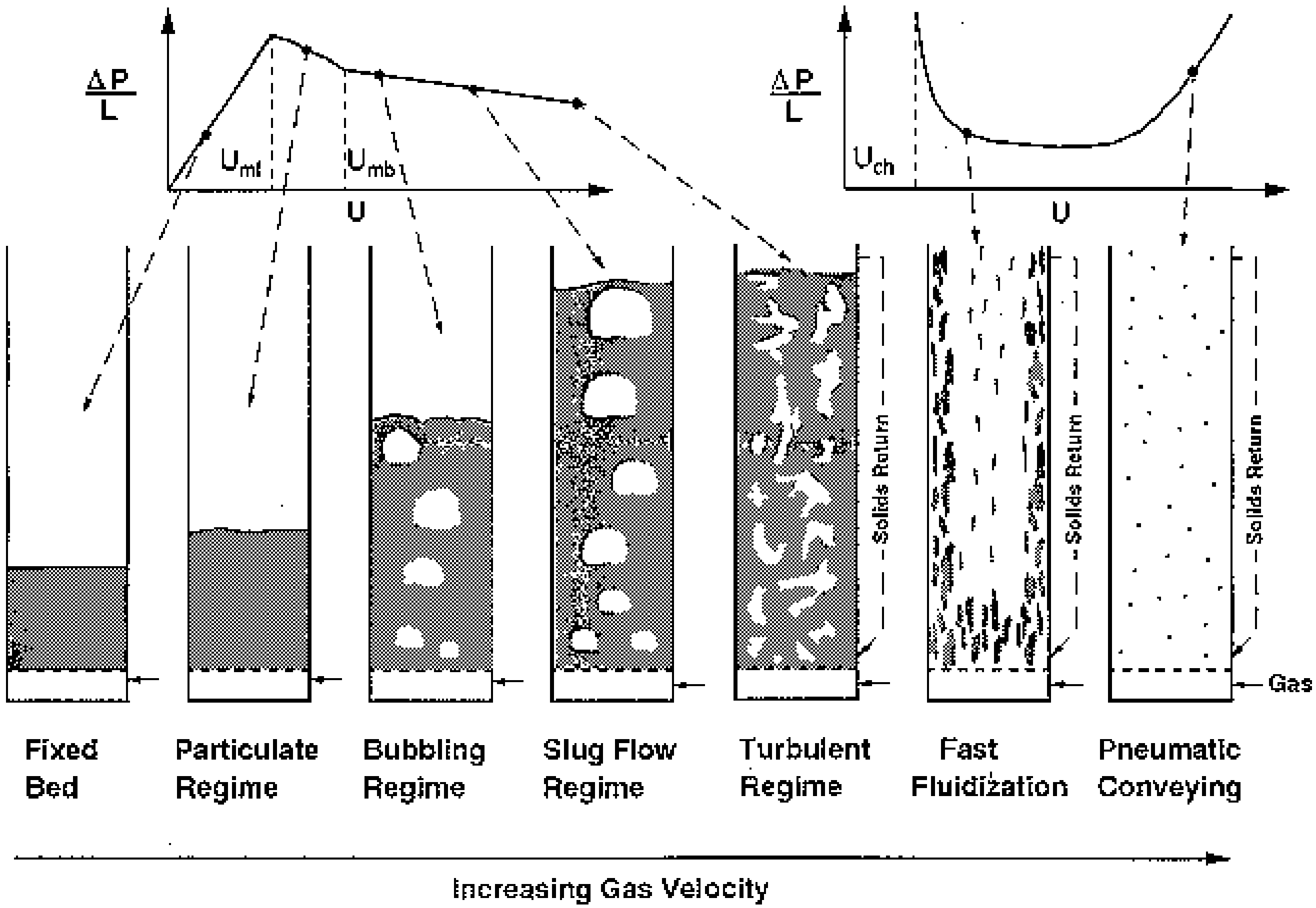
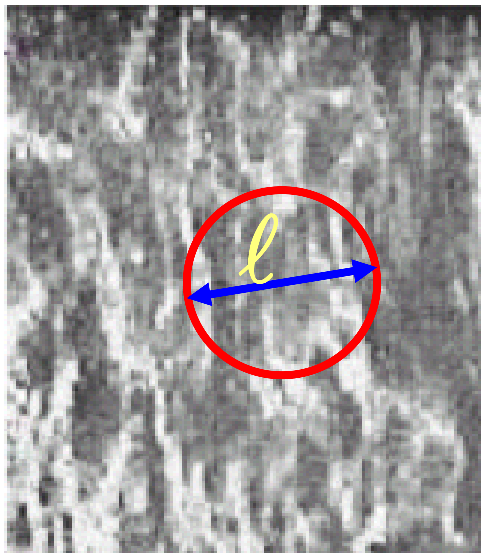
Sofiane Benyahia (Fluent)

FLUIDIZATION REGIMES



Averaged equations of motion: uniformly sized particles



Local-average quantities

- Phase volume fractions, ϕ_s, ϕ_f
- Particle phase velocity, $\langle \boldsymbol{u}_s \rangle$
- Fluid phase velocity, $\langle \boldsymbol{u}_f \rangle$

$$\phi_s + \phi_f = 1$$

Assume:

$$d \ll \ell \ll L$$

Does it make sense to talk of 2-D?

Energy flow in this problem

- Mean flow to fluctuating flow through fluid-particle slip forming small scale structures
- Coalescence and breakup of the structures
- This path exists in 2-D itself
- So, only quantitative differences between 2-D and 3-D, but not qualitative

Dependence of the filtered drag coefficient on resolution (2-D)

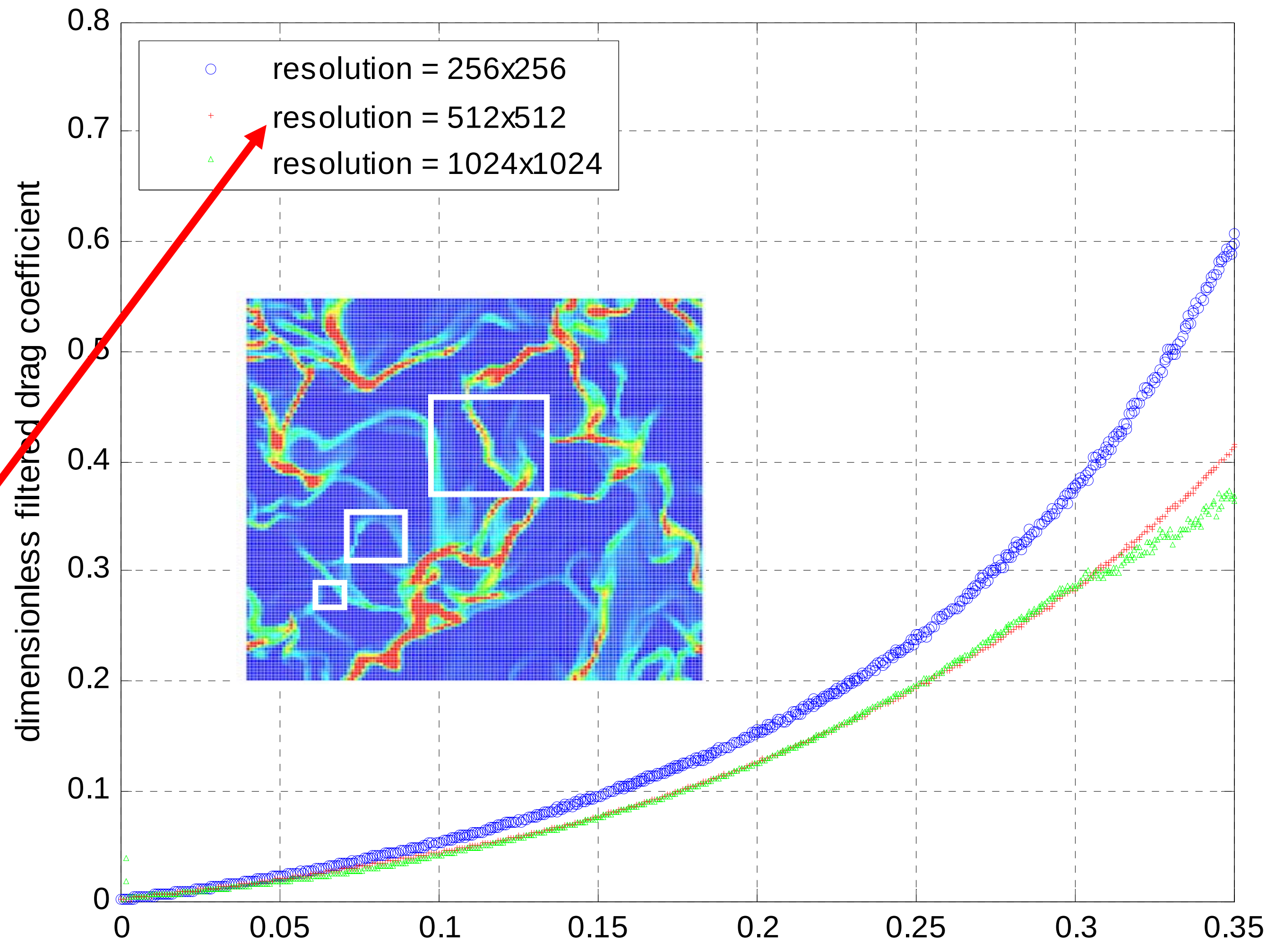
Domain size

= 64 x 64

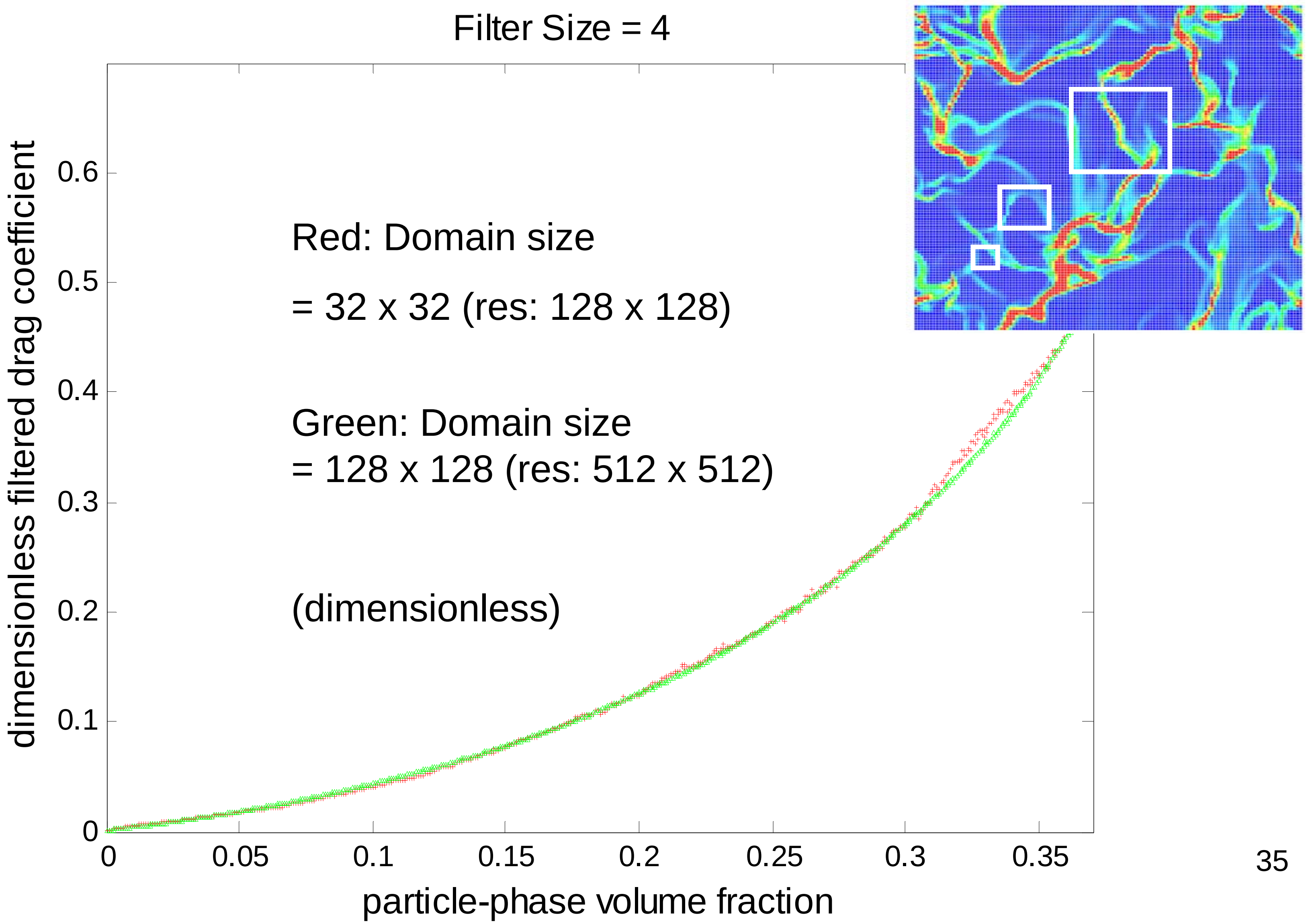
Filter size = 4

(dimensionless)

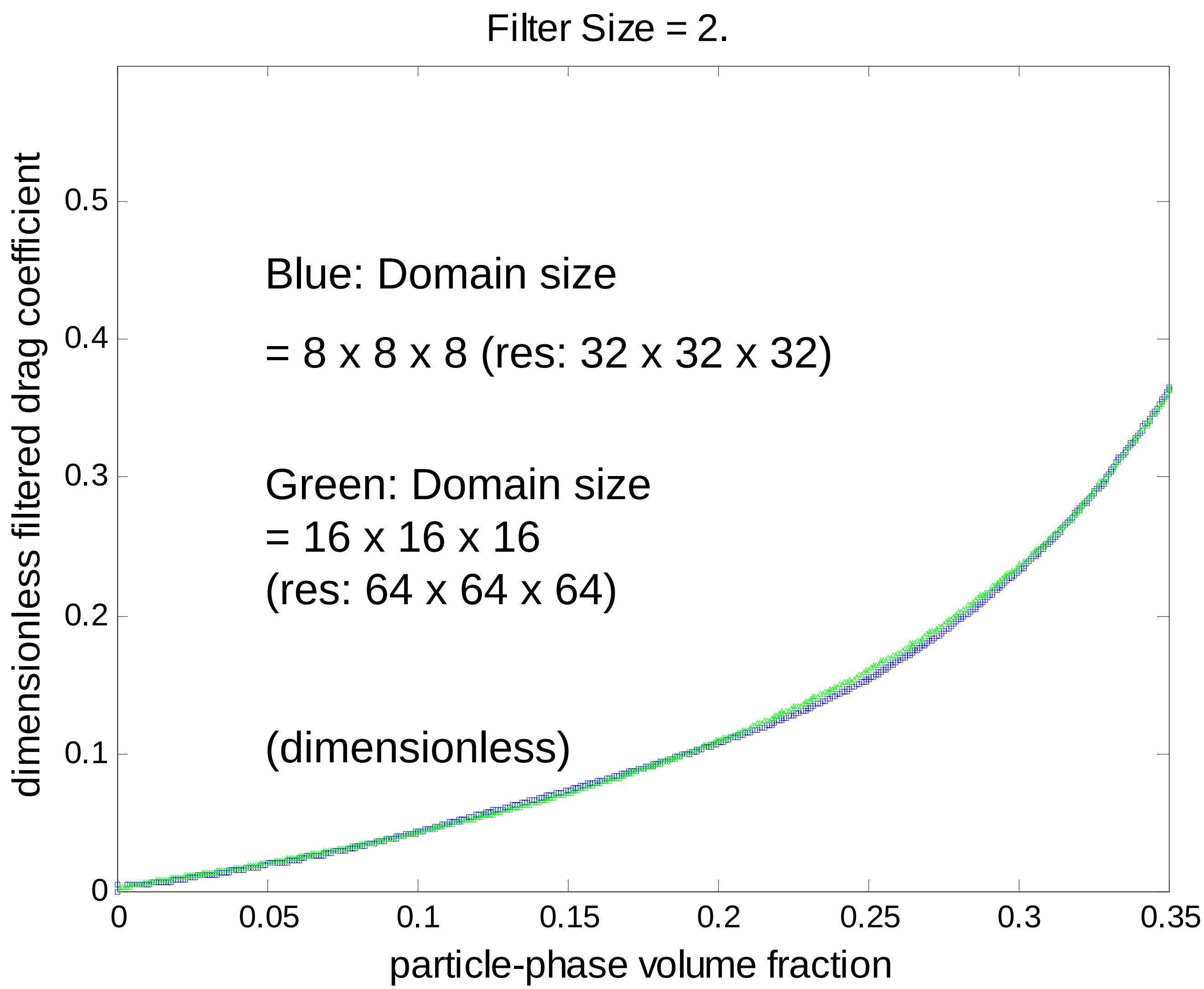
Corresponds to 1/8 cm



Filtered drag coefficient is independent of domain size (2-D)

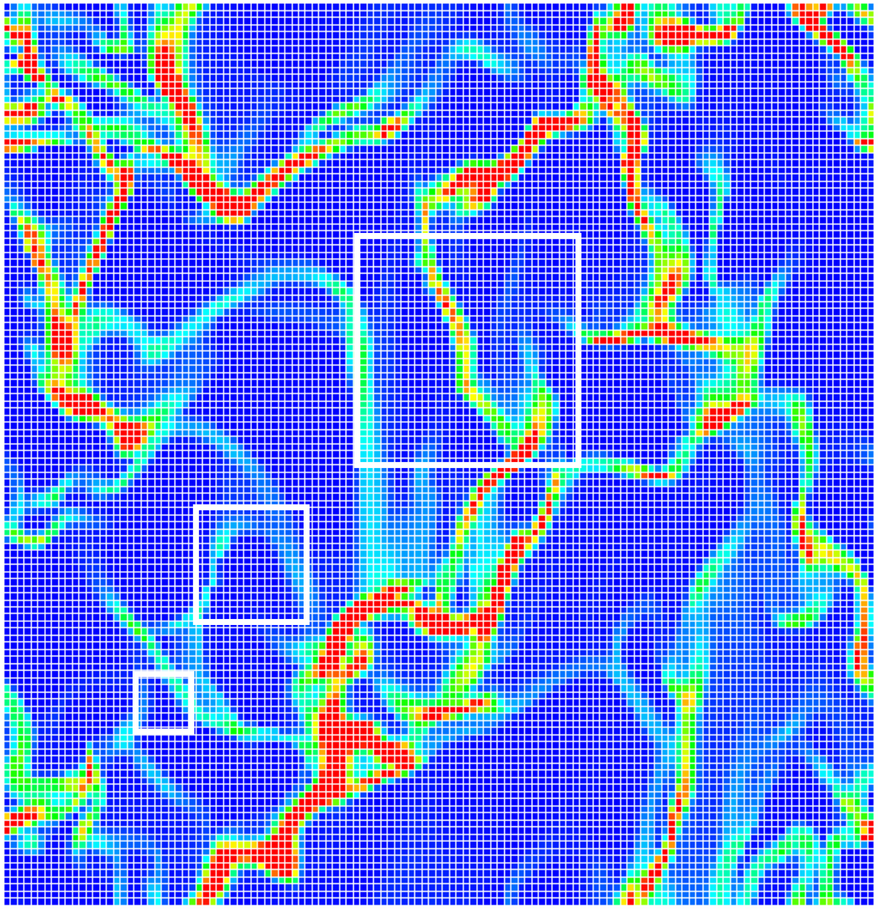


Filtered drag coefficient is independent of domain size (3-D)

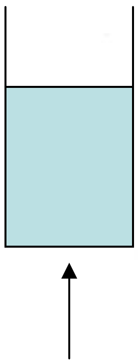


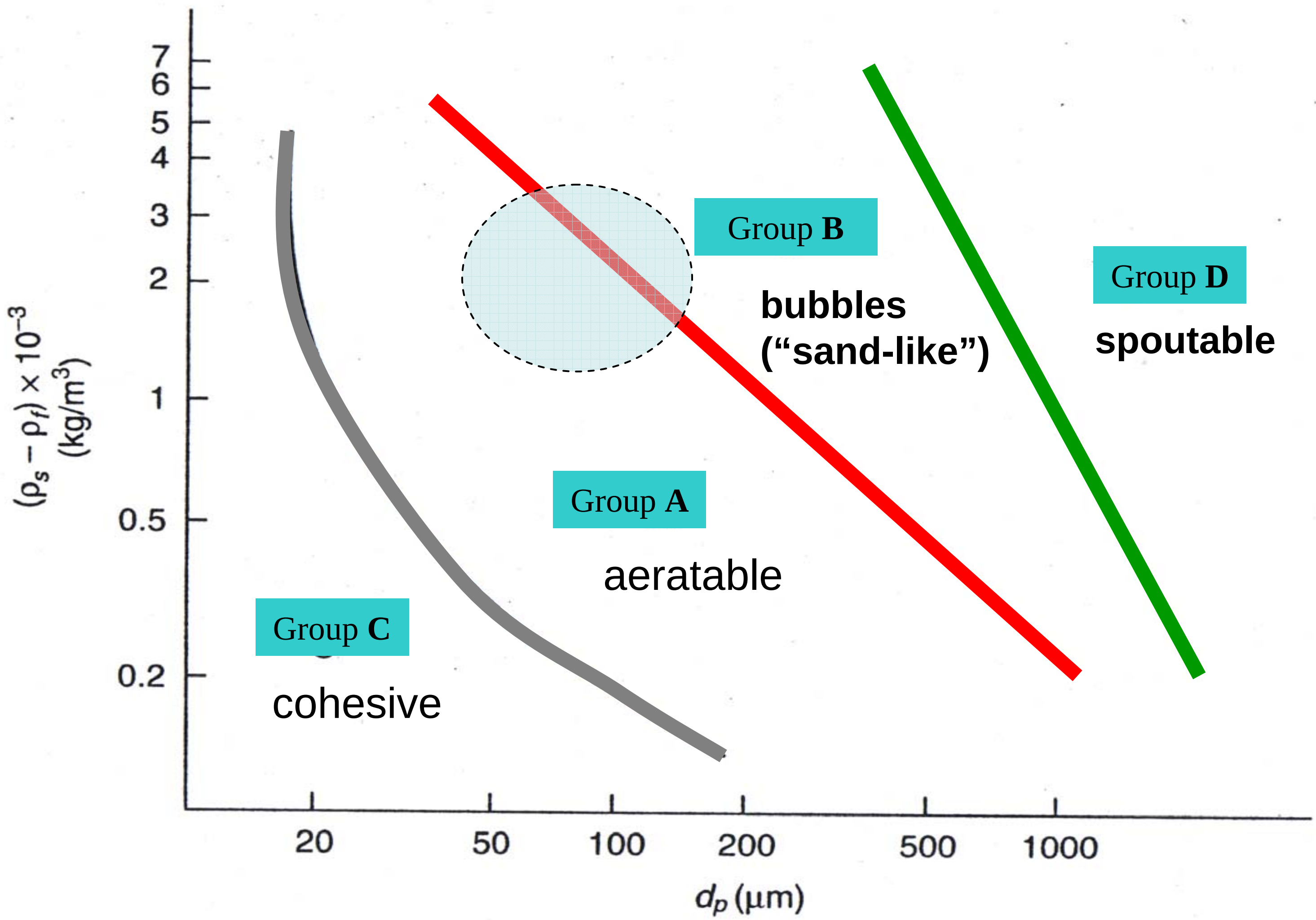
Filter "data" generated through highly resolved simulations of two-fluid models

Snapshot of particle volume fraction fields obtained in highly resolved simulations of gas-particle flows. Red color indicates regions of high particle volume fractions. Squares of different sizes illustrate regions (i.e. filters) of different sizes over which averaging over the cells is performed.



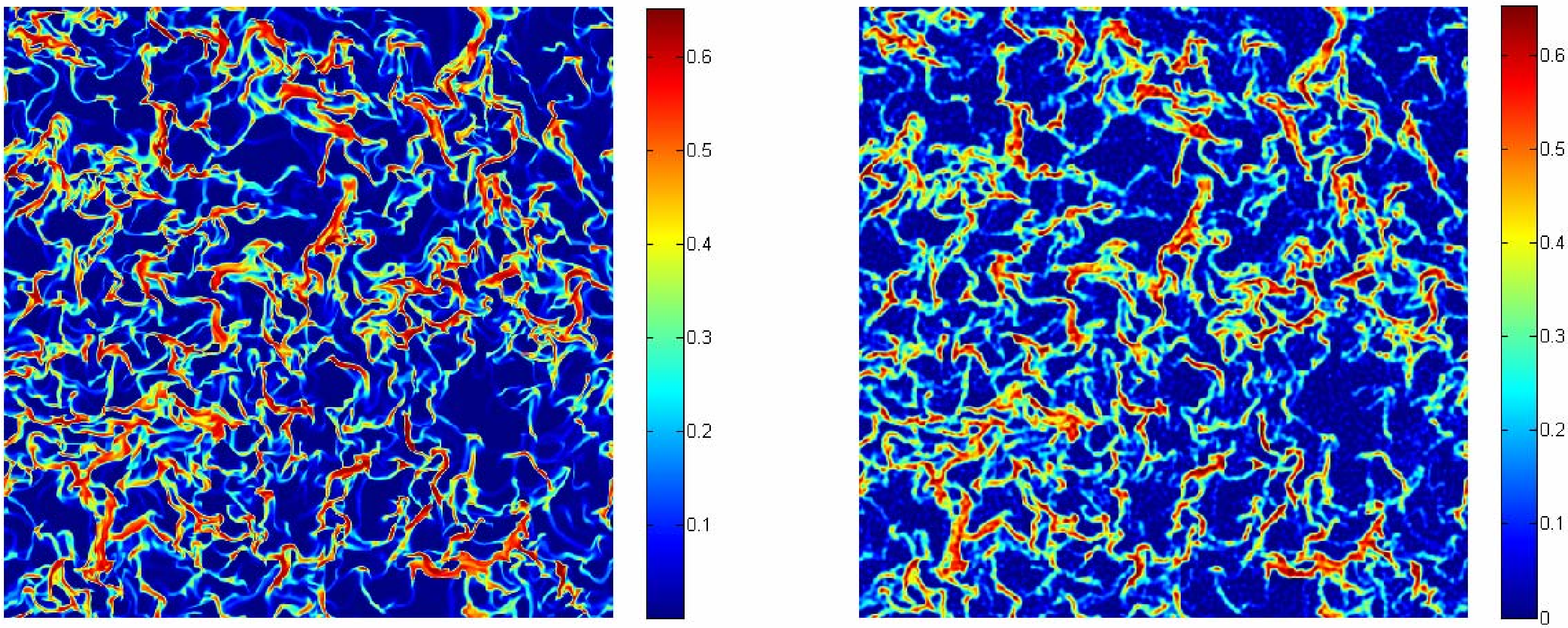
Geldart's Classification





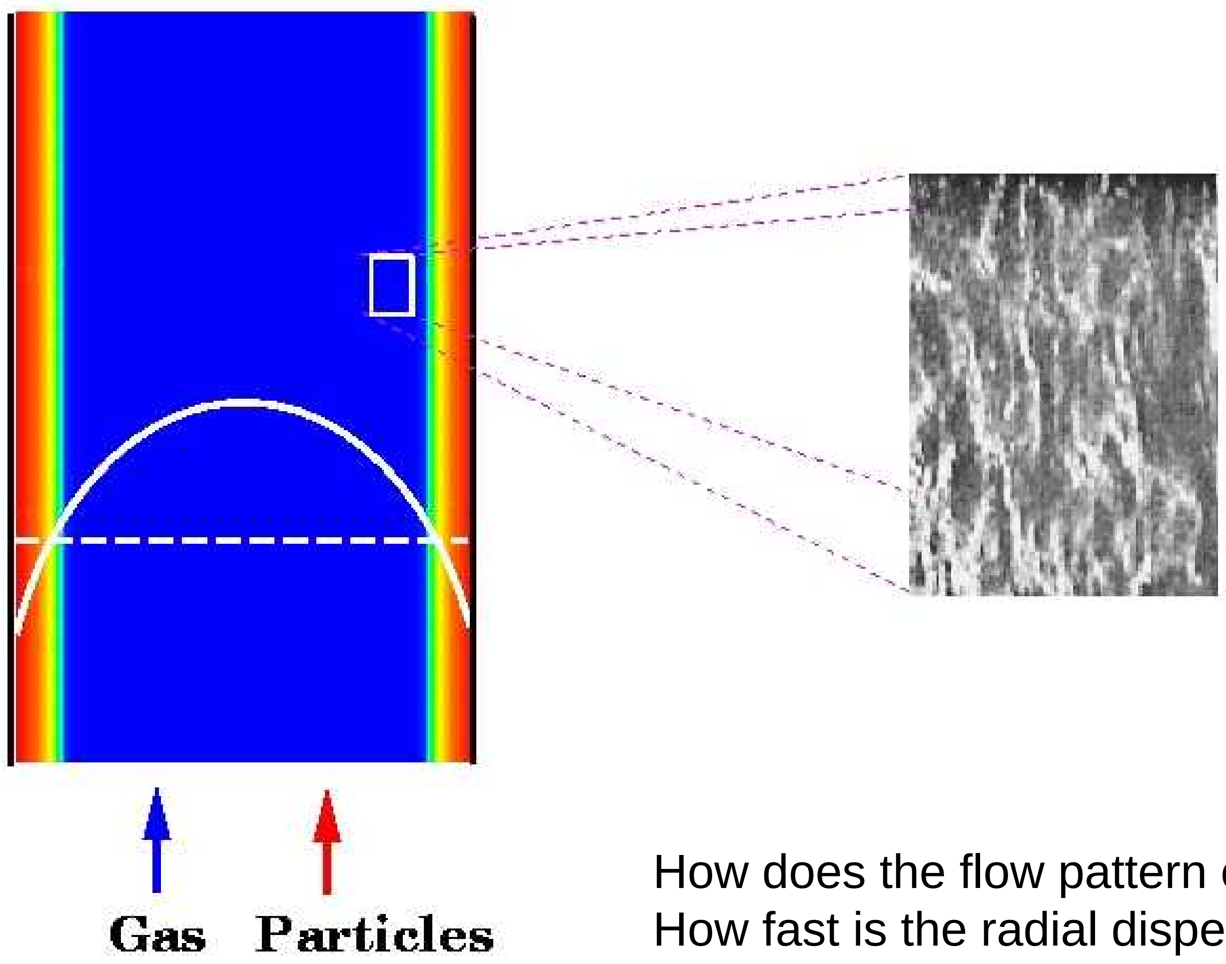
* **Geldart, Powder Tech. 7, 285 (1973).**

Kinetic Theory Model



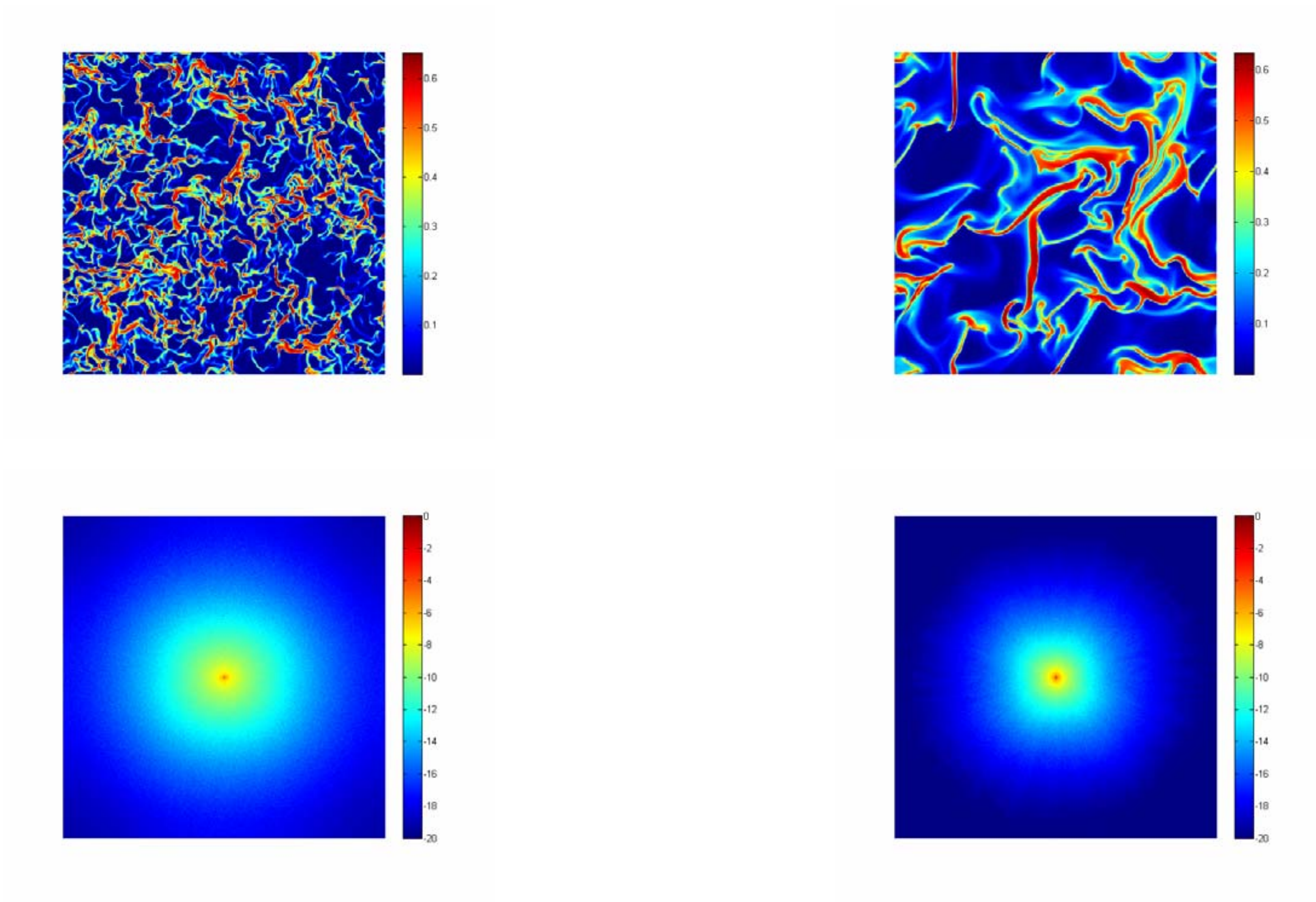
Reconstruction with $(\frac{a_{i,j}}{a_{\max}})^2 \geq 10^{-5}$

Flow behavior in fast fluidized bed/riser



How does the flow pattern change with scale up?
How fast is the radial dispersion?

Comparison of the kinetic theory and filtered models



64 cm x 64 cm, 512 x 512 grids